Format Specifications for Abstract Submission for the Fifteenth Symposium on Thermophysical Properties

Abstracts of 200-300 words must be submitted by **December 6, 2002**.

The content of the abstracts will be the basis for acceptance of papers for presentation at the symposium.

The abstracts should be submitted using the abstract-submission form on the Fifteenth Symposium website at http://symp15.nist.gov.

IMPORTANT: The online form will only accept ASCII characters. If your abstract uses special symbols, or includes equations, they will be lost when you paste your abstract into the form. However, in order to accomodate the most common cases of special symbols, namely superscripts, subscripts, and Greek letters, you can insert them into the form using a special (simple) syntax explained in a one-page PDF document: "How To Insert Symbols," available online. If you feel you *must* use either other symbols, or equations, then you *must* submit your abstract as an MS WORD file, using *only* US fonts (including symbols from any US font subset such as Latin-1 or Basic Greek), and following the format specifications given below. *Abstracts that do not conform to this format will not be accepted!* Abstracts submitted using the online form will *automatically* be formatted to conform to these requirements. Two MS Word files containing example abstracts are also available for download. (These are the example abstracts shown below.) Note that superscripts used to denote author affiliations are inserted automatically when you use the form, so no special handling is required.

We strongly recommend that you aviod using non-ASCII symbols, and that you avoid including equations in your abstract. *Figures cannot be included in abstracts.*

If you cannot use the online form, please send your abstract in MS Word to the symposium email address: symp15@boulder.nist.gov, as an attachment. The main email message to which the abstract is attached should indicate:
(a) preference for poster or oral presentation;
(b) the most appropriate special or general session(s);
(c) the speaker;
(d) the corresponding author (including e-mail address as well as telephone and fax numbers).

We will attempt to honor your requests for items (a) and (b), but adjustments may be required for the organization of the Symposium. Final assignments of each paper will be included in the acceptance letter.

Please refer to the examples at the end of this document to clarify the instructions below.

Font: All text is Times New Roman. The title is 11 point, authors and their affiliations are 10.5 point, and body text is 10 point.

Title: The title should be Bold, Centered, and start all major words with Capital letters (other than words like “of”, “and”, “or”, “in”, etc.)

Author(s): The list of authors should be Centered, names of multiple authors with a common affiliation are separated by commas, with “and” used before the last author. For each author list first and middle initials, followed by last name spelled out – no spaces between multiple initials, one space separating leading initials from last name (surname). Authors’ affiliations begin immediately on the following line. One blank line (double line-space) separates author information for authors with different affiliations. The list of authors should indicate the author to whom correspondence should be addressed with a

superscript C following that author's name. The speaker should be indicated similarly, with a superscript S.

Author's Affiliation (Company/University): Affiliations should be Centered and Italicized, with complete addresses including Country. Continue on multiple lines as needed. Affiliations immediately follow on the next line after each author's name, or after a comma-separated list of authors sharing a common affiliation. The email address of the author to whom correspondence should be addressed (or an email address at which this author can be reached) should be included as the last line of that author's address.

In the unusual situation of multiple authors with the same affiliation, but who are not listed in order (that is, their names are separated by the names of other authors with different affiliations), superscript numbers (1,2,3, etc.) can be used to identify author affiliations. In this case, the different affiliations are written separated from the list of names and from each other by single blank lines (double line-space), with each affiliation preceded by its corresponding number (as a superscript). These affiliations should be numbered in order, 1,2,3, etc.

Body Text: Text should be full block, single-spaced paragraphs, with no tabs, and double-spacing between paragraphs. Single spaces should be used between sentences, after each period. The text should be fully justified.

References: Sequential references are indicated in the text by numbers in square brackets, for example [1]. All references are listed at the bottom, separated from the abstract by a single blank line (double line-space), again with numbers in square brackets. The first author's name should be three spaces from the reference number. If text wraps to a second line, this line should be tabbed to the same tab stop as the first author's name, so that it lines up under that name. Authors' names are listed using first and middle initials, followed by last name spelled out – no spaces between multiple initials, one space separating leading initials from last name (surname). Authors are separated by commas, with ", and" used before the last author, and a comma following the last author. This is followed by the *Journal Name* in italics, a single space with no comma, the **Volume** number in bold followed by a comma, the initial page number, a single space with no comma, the year in parentheses, and ending with a period.

Footnotes: Use superscript symbols rather than numbers. Separate footnotes from last line of text by triple line-space. In general, the use of footnotes in abstracts is discouraged.

Equations: Equations should not be numbered. Equations should use only the standard symbol set from the U.S. English version of Word. *This is very important!* The use of other symbols may result in their not being properly displayed in the typeset version (since they may not be available to us.) In general, the use of equations in abstracts is discouraged.

Paper: - A4 (8.27 x 11.69 inches)

Margins: - 1 inch for top and sides

An example abstract showing the desired format is shown on the next page.

Critical Fluctuations and G^E-Models for Ternary Mixtures

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Phase equilibria in ternary mixtures have an immense importance in technological processes, like separation, extraction and particle formation. Several models were developed to describe the phase behavior of ternary systems. Based on the excess Gibbs-energy representation, all models are mean-field in essence, i.e., they neglect the effect of critical fluctuations on the thermodynamic behavior and, therefore, they give incorrect results near critical points.

Recently, Anisimov, Sengers and collaborators[1,2] have developed a crossover theory that incorporates the correct asymptotic critical behavior and crosses over to mean-field behavior. Moreover, they used their crossover theory to include the effect of critical fluctuations in prototypical classical equations (van der Waals equation for one-component [3], NRTL equation for binary liquid-liquid equilibria [4]). In this paper we discuss the extension of the Anisimov and Sengers crossover theory (ASXT) to ternary systems. In order to apply ASXT, a thermodynamic potential that is isomorphic with the one-component Helmholtz-energy is required. For that purpose, a Legendre transformation of the Gibbs-energy defines the grand-potential $\Omega(T,x_2,\mu_{13})$ which, after minor changes in variables, allows the description of the ternary systems. The discrepancy between independent variables of G^E $(T,\{x_i\})$ models and of the isomorphic thermodynamic potential $\Omega(T,x_2,\mu_{13})$ is solved in an iterative way. The procedure is applied to simple G^E models. Impurity effects in binary systems, phase behavior of solid-saturated solutions in mixtures of two solvents are discussed.

[1] Z.Y. Chen, P.C. Albright, and J.V. Sengers, *Phys. Rev. A* **41**, 3161 (1990); G.X Jin, S. Tang, and J.V. Sengers, *Phys. Rev. E* **47**, 388 (1993).
[2] M.A. Anisimov, S.B. Kiselev, J.V. Sengers, and S. Tang, *Physica A* **188**, 487 (1992).
[3] A. Wyczalkowska Kostrowicka, M.A. Anisimov, and J.V. Sengers, *Fluid Phase Equil*. **158**, 523 (1999).
[4] T.A. Edison, M.A. Anisimov, and J.V. Sengers, *Fluid Phase Equil*. **150-151**, 429 (1998).

An example abstract showing an alternative format for references is shown on the next page. This alternative format should be avoided if possible.

Solid-Liquid Equilibrium of Hard Dumbbells with Dipoles and Quadrupoles: Application to Methyl Chloride

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We calculate the solid-liquid equilibrium of a system of hard dumbbells with embedded point dipoles and quadrupoles in a generalized van der Waals theory. This work is an extension of earlier calculations for the purely dipolar system. The molecular parameters are chosen to approximate a system of methyl chloride molecules. The solid free energy is calculated by using the simple cell theory of Lennard-Jones and Devonshire to approximate the free energy of the hard-dumbbell solid with the multipole contributions to the free energy approximated by static lattice sums of the pair interactions. Two different crystal structures are considered as candidates for the structure of the solid at freezing, one of which is close packing. Thermodynamic perturbation theory is used to add dipole-dipole, dipole-quadrupole, and quadrupole-quadrupole interactions to the equation of state of the hard-dumbbell fluid. For the hard-dumbbell equation of state, we use that of Maeso and Solana. We carry out new Monte Carlo simulations to characterize the accuracy of the perturbation theory. Application of the Maxwell double-tangent construction yields the phase equilibrium between the solid and liquid. We are able to calculate the effect of molecular dipole and quadrupole moments on the phase diagram of the system of dumbbells. In particular, we examine the effects of the multipoles on the stable crystal structure at freezing, the ratio of triple point temperature to critical point temperature, and the density change at freezing.

NOTE: This abstract could be submitted using the web form, but serves to illustrate the format.